

## **Supplemental Information**

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Number of tables: 3

## Methods

### *Tapwater Sampling for VOCs*

Samples were collected in dechlorination sample bottles containing 25 mg ascorbic acid. Water samples were collected from cold water kitchen taps without faucet treatment devices. Aerators were removed when feasible. Water was flushed at laminar flow for ten seconds prior to sample collection to ensure that the sample came from household pipes, not the faucet, service line or water main. Samples were collected from the flowing stream. The pH was adjusted to  $< 2$  at the time of collection, but after dechlorination, by adding two drops of 1:1 HCl for each 40 mL of sample. Then the sample was transferred into three 40 mL sample bottles. Bottles were filled to obtain a reverse meniscus and capped ensuring no air bubbles passed through as the bottle was filled, or were trapped in the sample when the bottle was sealed. Samples were placed into two self-closing plastic bags, placed on ice in a cooler lined with plastic bags, and delivered by same-day courier to BC Laboratories, Inc., Bakersfield, CA for analysis using gas chromatography/mass spectrophotometry, according to EPA Method 524.2 for 103 VOCs.<sup>i</sup> Samples from November 2019 were collected in duplicate and the second set was sent to Excelchem Environmental Labs, Rocklin, CA by courier for analysis using the same testing method. All samples were analyzed within 14 days of collection. Trip blanks, field blanks, and temperature blanks were included with each shipment. Temperature blanks confirmed that all samples were maintained at 4°C until analysis. Of the 29 field and trip blanks collected in the October sampling trip, 17 contained low levels of acetone or chloroform. Two blanks each contained traces of toluene, isopropanol, or MeCl. Acetone and chloroform were excluded from further analysis. Toluene and isopropanol were not found in tap water samples and were therefore also excluded. The two blanks with MeCl were only slightly above the practical quantitation limit (PQL) of 0.5 micrograms per liter (ug/L). All blanks collected during the November sampling period had no VOCs detected.

### *Tapwater Non-Targeted Analysis*

Water samples (2.5 L) were collected in an amber glass jar and passed over an Oasis HLB cartridge (Waters, Massachusetts, USA) to enrich compounds with a broad range of octanol-water partition coefficients ( $K_{ow}$ ). A minimal amount of sodium sulfate was added to the jar to collect residual water, and the jar was rinsed with 3 x 4 mL hexane/acetone (3:1 v/v) to recover compounds adsorbed to the container. Cartridges were dried for at least one hour prior to extraction. Once dry, cartridges were eluted with 2 x 5 mL ethyl acetate followed by 2 x 5 mL methanol. The ethyl acetate portion was combined with the jar rinse, and both ethyl acetate and methanol eluates were evaporated to 1 mL with nitrogen using a Turbovap (Biotage). Half of the ethyl acetate extract was combined with half of the methanol extract. The combined extract was evaporated to 200  $\mu$ L and spiked with dibromooctafluorobisphenol (DBOBF, 10 ng) as an internal standard. As a quality check on the non-targeted method, a calibration curve for selected semivolatile organic compounds (SVOCs) consisting of thirteen points between 0.1 – 1000 ng/mL was prepared in ethyl acetate, spiking internal standard at the same concentrations as the samples. Analysis was performed using a gas chromatograph coupled with a quadrupole time-of-flight mass spectrometer (GC-QTOF-MS; Agilent 7890B GC coupled to an Agilent 7200B QTOF-MS with a HP-5MS UI 30 m x 0.25 mm, 0.25  $\mu$ m column, Agilent Technologies, Inc.) operated in electron ionization mode. All acquired data files were deconvoluted and aligned using MS-

DIAL v. 3.90.<sup>ii</sup> Compound identification was conducted by matching EI spectra and retention indexes against compounds found in the NIST17 mass spectral database, with tentative identification reported for compounds with match scores above 70; confirmed identifications are only available for the compounds included in the target analysis method.

Figure S1: Paradise Irrigation District's service boundary and sampled service lateral locations showing estimated odds ratio of intensities for locations that detected benzene (red circles) compared to locations with no benzene detections (grey open circles). Intensity ( $s$ ) represents the expected number of events per unit area at location  $s$ . Color gradient indicates the ratio of intensity where yellow is high, and blue is low.

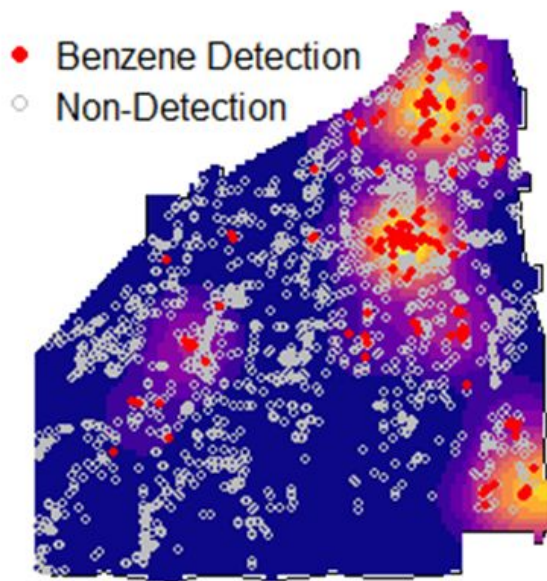


Figure S2. Target semivolatile organic compound concentrations with the most frequent detections in the nontarget analysis subset of samples. Phenol concentrations are divided by 10 to facilitate depiction on the same scale.

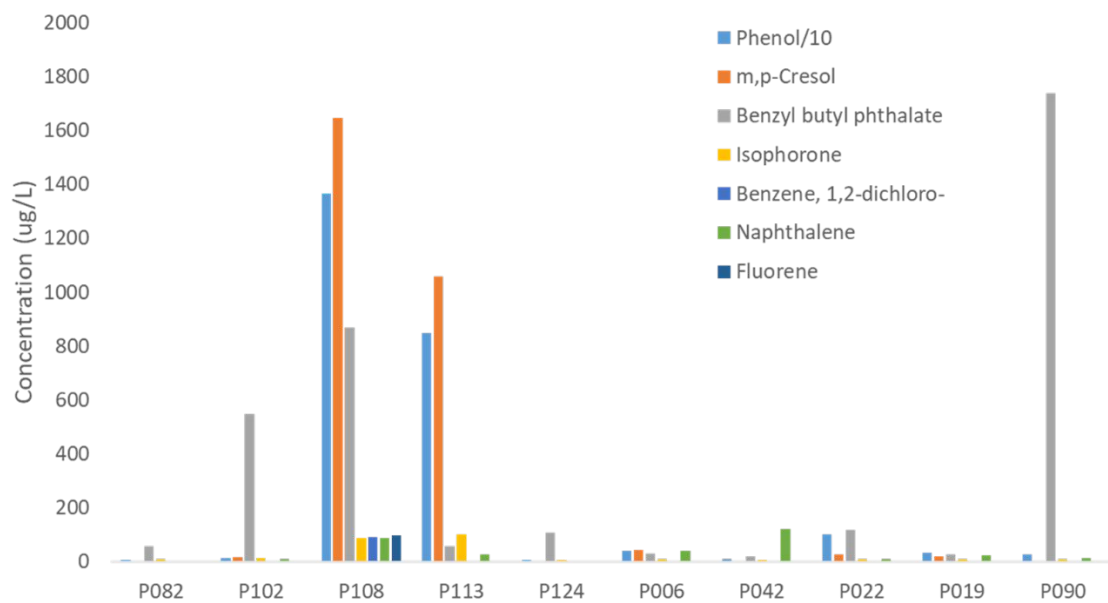


Figure S3. Illustration of the nontarget feature alignment and identification process in MS-DIAL for the nontarget feature bromodichloromethane. The linear correlation coefficient between the nontarget feature identified as bromodichloromethane with the concentration measured independently during the VOC analyses was 0.75.

Chromatograms in an aligned spot: double click to modify the peak areas.

File ID	File Name	Peak ID	Class	Annotation	TotalScore	Rt	RJ	S/N	Peak Int.	Peak Area	Chromatogram
3	200106_20_P102_Paradise_101619_EI	26	1	Methane, bromodichloro-	956.71	5.26	691.6	220.5	1701211	4164746	
2	200106_19_P082_Paradise_101619_EI	24	1	Methane, bromodichloro-	909.14	5.24	690.9	279.7	1544376	3746330	
6	200106_23_P124_Paradise_101619_EI	21	1	Methane, bromodichloro-	941.05	5.15	687.4	227.8	1114140	2662382	
9	200106_27_P042_Paradise_111919_EI	22	1	Methane, bromodichloro-	950.81	5.20	689.3	225.2	986825	2550953	
4	200106_21_P108_Paradise_101619_EI	17	1	Methane, bromodichloro-	905.50	5.24	691.0	22.1	771443	1865174	
8	200106_26_P006_Paradise_111919_EI	23	1	Methane, bromodichloro-	929.69	5.23	690.5	133.6	692374	1695364	
10	200106_28_P022_Paradise_111919_EI	21	1	Methane, bromodichloro-	949.72	5.24	691.1	104.8	578909	1437074	
12	200106_30_P090_Paradise_111919_EI	19	1	Methane, bromodichloro-	941.84	5.17	688.3	73.8	505969	1300167	
11	200106_29_P019_Paradise_111919_EI	19	1	Methane, bromodichloro-	919.46	5.18	688.8	34.5	177224	456517	
5	200106_22_P113_Paradise_101619_EI	25	1	Methane, bromodichloro-	926.92	5.29	692.9	15.9	96655	229313	
7	200106_25_mtdbik_Paradise_111919_EI	-2	Method Blank		-1.00	5.21	690.0	0.2	1919	5980	
1	200106_18_mtdbik_Paradise_101619_EI	-2	Method Blank		-1.00	5.28	692.5	0.2	1684	4944	
0	200106_12_STD100_Megamix_EI	-2	Megamix		-1.00	5.24	691.2	0.0	93	467	
13	200106_31_STD100_Megamix_EI	-2	Megamix		-1.00	5.21	689.8	0.0	86	382	
14	200106_32_STD100_Ext_hyd_EI	-2	Ext Hyd		-1.00	5.19	689.2	0.0	90	358	

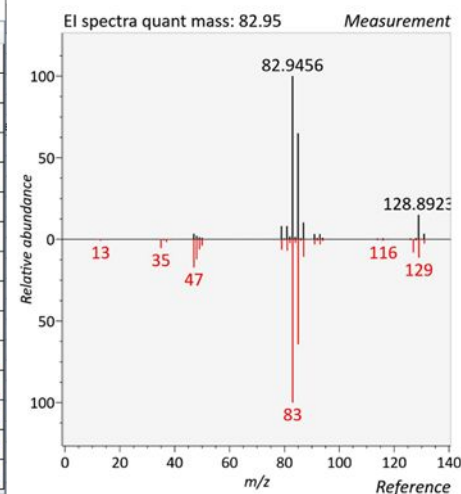
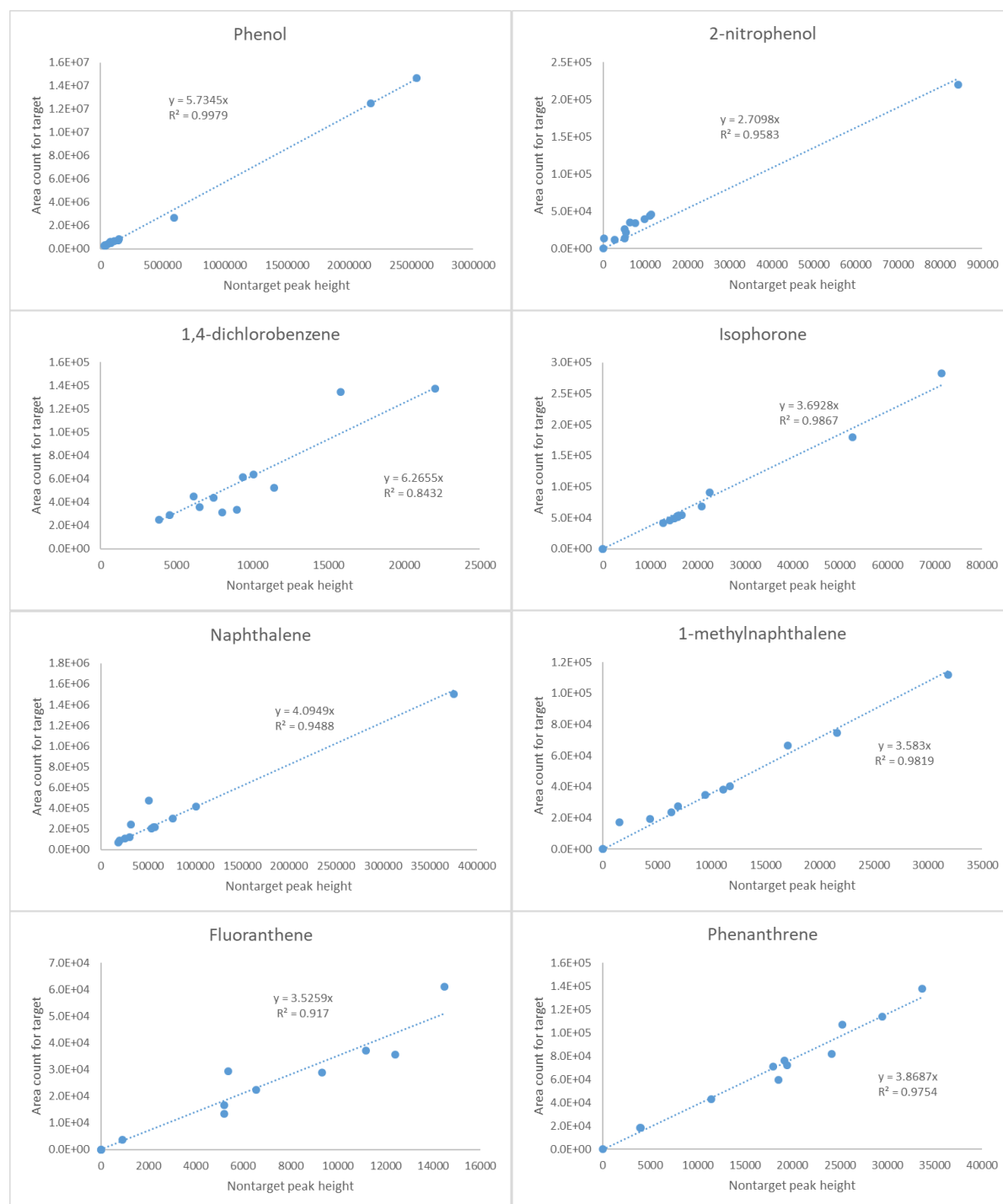


Figure S4. Comparison between nontarget peaks identified as target compounds and the corresponding area counts used in quantifying the targets obtained independently from the same data set. Note that for some of these compounds, all samples were below the formal method detection limit for the target compounds (2-methylnaphthalene, 1,4-dichlorobenzene, fluoranthene) and for others most of the samples were below the MDL (Table S2).



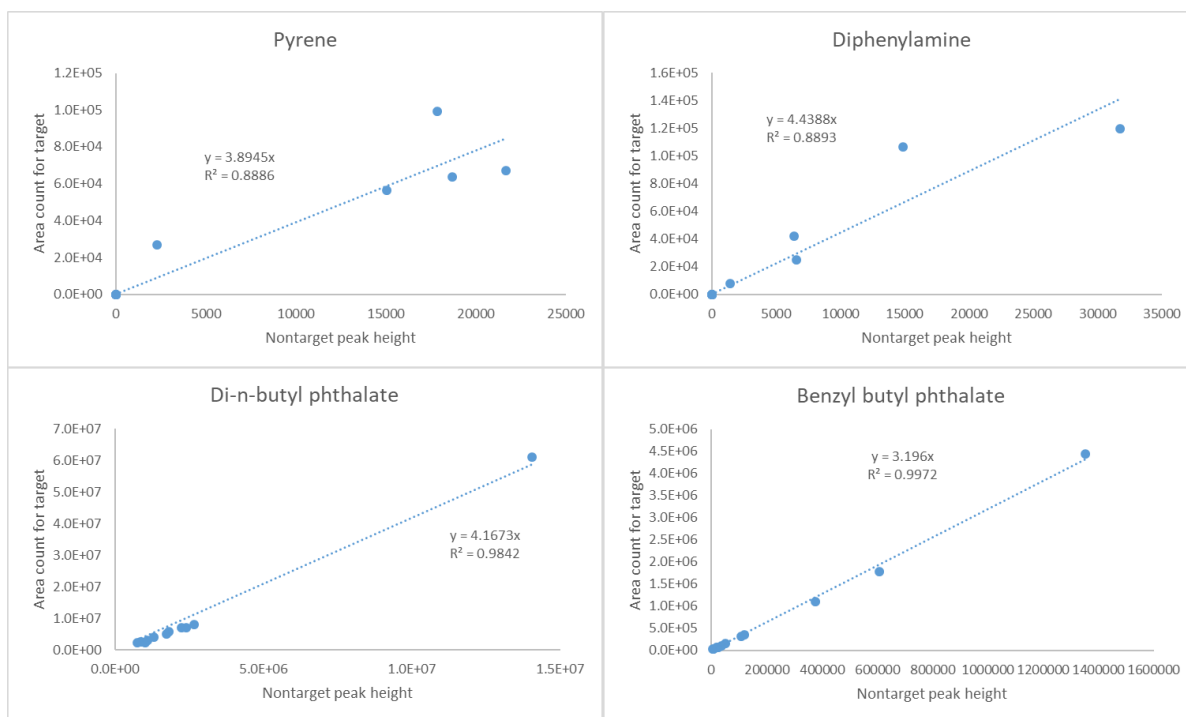


Figure S5. Principal components analysis using aligned nontarget GC-QTOF-EI data for the 10 household samples (gold symbols), the two method blank samples (red symbols) and the analytical standard used for quantification and retention index calibration (turquoise symbols).

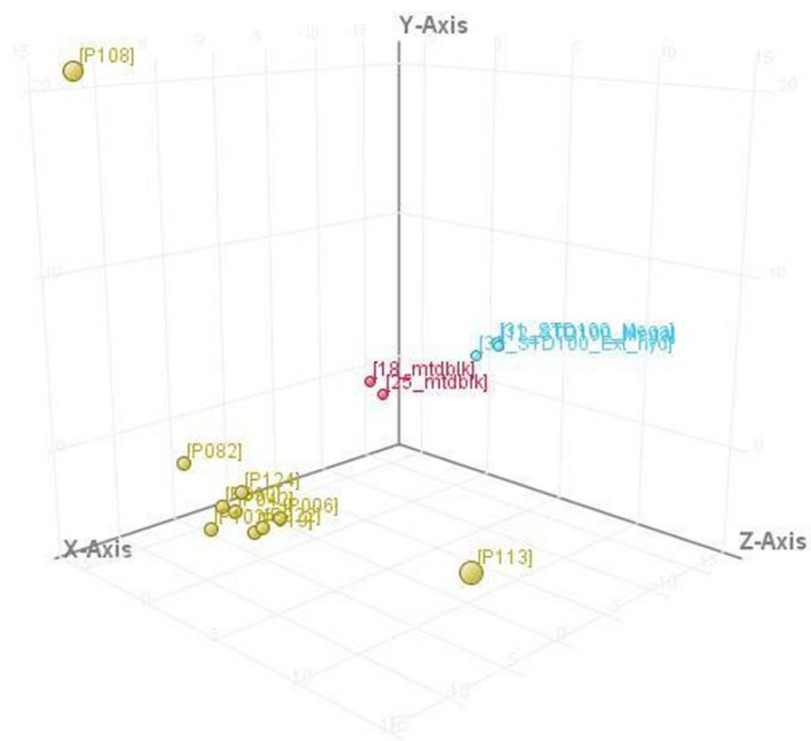


Figure S6. Hierarchical cluster analysis of the aligned GC-QTOF-MS feature heights for the 10 household samples, two method blank samples and three analytical standards used during the nontarget analysis component of the project.

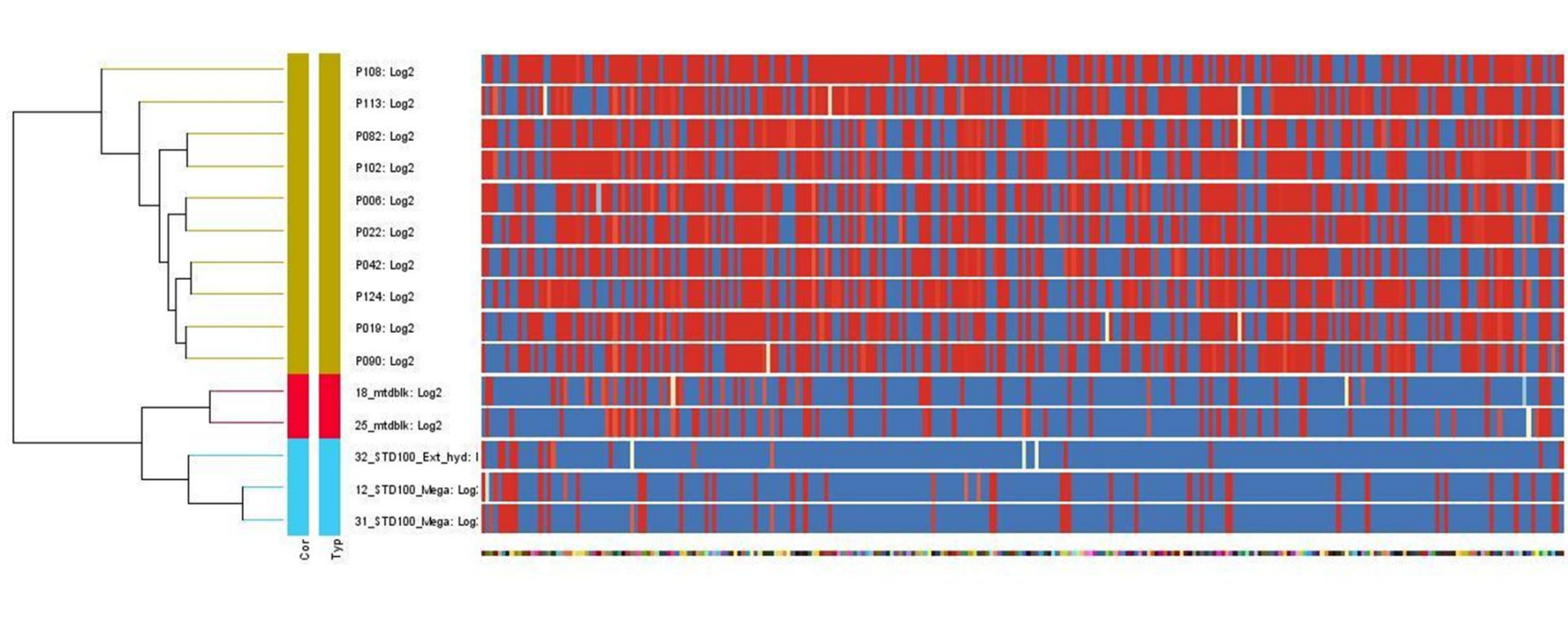


Table S1. Semivolatile Organic Compounds (SVOCs) included as targets in the nontarget analysis that had no detections in the 10 homes sampled for nontarget analysis and their associated limits of detection.

Compound	LOD (ng/mL)
1,2,4-Trichlorobenzene	10
1-Methylnaphthalene	5
2-Methylnaphthalene	50
4-Bromophenyl phenyl ether	10
4-Chlorophenyl phenyl ether	25
Acenaphthene	5
Acenaphthylene	10
Anthracene	25
Benz(a)anthracene	10
Benzene, 1,3-dichloro	5
Benzene, 1,4-dichloro	250
Benzene, hexachloro-	2.5
Benzene, nitro-	100
Benzo(a)pyrene	25
Benzo(b)fluoranthene	25
Benzo(g,h,i)perylene	25
Benzo(k)fluoranthene	25
Bis(2-chlorethoxy)methane	50
Bis(2-ethylhexyl) adipate	250
Bis(2-ethylhexyl) phthalate	>1000
Carbazole	50
Chrysene	50
Dibenz(a,h)anthracene	50
Dibenzofuran	10
Di-n-butyl phthalate	>1000
Fluoranthene	5
Hexachlorobutadiene	5
Indeno[1,2,3-cd]pyrene	25
Naphthalene, 2-chloro-	10
Phenanthrene	10
Phenol, 2,4-dichloro	250
Phenol, 2,4-dimethyl-	100
Phenol, 2-chloro-	100

Table S2. Semivolatile Organic Compounds (SVOCs) included as targets in the nontarget analysis that had at least one detected concentration above the method detection limit (LOD) in the 10 homes sampled for nontarget analysis and their associated limits of detection.

Compound	MDL (ug/L)	Method Blank Oct	Method Blank Nov	P082 Oct	P102 Oct	P108 Oct	P113 Oct	P124 Oct	P006 Nov	P042 Nov	P022 Nov	P019 Nov	P090 Nov
Di-n-octyl phthalate	50		<MDL	<MDL	<MDL	64.8	52.2	<MDL	55.4	<MDL	55.3	58.4	53.2
Benzyl butyl phthalate	100	<MDL	<MDL	<MDL	546.9	868.1	<MDL	108.1	<MDL	<MDL	118.2	<MDL	1738
Isophorone	10			<MDL	13.8	88.2	102.1	<MDL	<MDL	<MDL	10.5	<MDL	<MDL
Ethane, hexachloro-	5			25.6	12.2			9.8					<MDL
Phenol	1000	<MDL	<MDL	<MDL	<MDL	13650	8490	<MDL	<MDL	<MDL	1007	<MDL	<MDL
Hexachlorocyclopentadiene	100			170.1	151.5	<MDL		<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
m,p-Cresol	250				<MDL	1648	1059		<MDL		<MDL	<MDL	
Naphthalene	50	<MDL	<MDL	<MDL	<MDL	87.2	<MDL		<MDL	119.8	<MDL	<MDL	<MDL
Benzene, 1,2-dichloro-	25	<MDL				88.7	<MDL			<MDL	<MDL	<MDL	
Diphenylamine	25				<MDL	52.1					<MDL		
Fluorene	5					98.5							
N-Nitroso-di-N-propylamine	50					299.5							
o-Cresol	100					205.0		<MDL	<MDL		<MDL	<MDL	
Phenol, 2-nitro-	500		<MDL			871.3			<MDL		<MDL	<MDL	<MDL
Pyrene	5						5.3						

<MDL Compound potentially present, but at a level below the formal method detection limit.

Blank cells indicate that there was no indication the compound was present in the sample.

**Table S3. Summary of the results of each filtering step applied during the nontarget workflow on the number of remaining molecular features**

Filtering Step	Number of Features Remaining
Total aligned features	1914
Detected in at least 1 household sample	1906
Maximum sample/average method blank > 10	1477
Average signal to noise > 20	509
Tentatively identified (NIST ID score > 70)	265

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<sup>i</sup> Budde W and Munch J. 1995. Methods for the Determination of Organic Compounds in Drinking Water –Supplement III. National Exposure Research Lab, Office of Research and Development, U.S. Environmental Protection Agency, Washington, D.C., EPA/600/R-95/131 (NTIS PB95261616). <https://nepis.epa.gov/Exe/ZyPDF.cgi?Dockkey=30003E77.PDF>

<sup>ii</sup> Tsugawa H, Cajka T, Kind T, Ma Y, Higgins B, Ikeda K, Kanazawa M, VanderGheynst J, Fiehn O, Arita M. 2015. MS-DIAL: data-independent MS/MS deconvolution for comprehensive metabolome analysis. **Nat Methods** 12(6):523-526, DOI: 10.1038/nmeth.3393.